Covariance and Other Nuclear Data in SCALE 6.3

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Outline

- Need for high-quality covariance data
- Brief history of covariance data in SCALE
- Updates pursued beyond just cross sections in SCALE 6.2
- Ramifications
- 6.3 Goals
  - delayed neutron uncertainty
  - sensitivity indices
  - improved infrastructure for covariance operations
  - on-the-fly sampling and correlated input sampling

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Need for high-quality covariance data

- S/U Tools in SCALE rely on reasonable estimates for nuclear data uncertainty
- Historical lack of sufficient covariance data in ENDF
  - Treated as zero uncertainty, can be viewed as lower bound estimate on unc.
  - Problematic for TSURFER – GLLS will adjust wrong data, compensate incorrectly
    - Onus on user to provide their own "reasonable" guess of what the unc. *should* be

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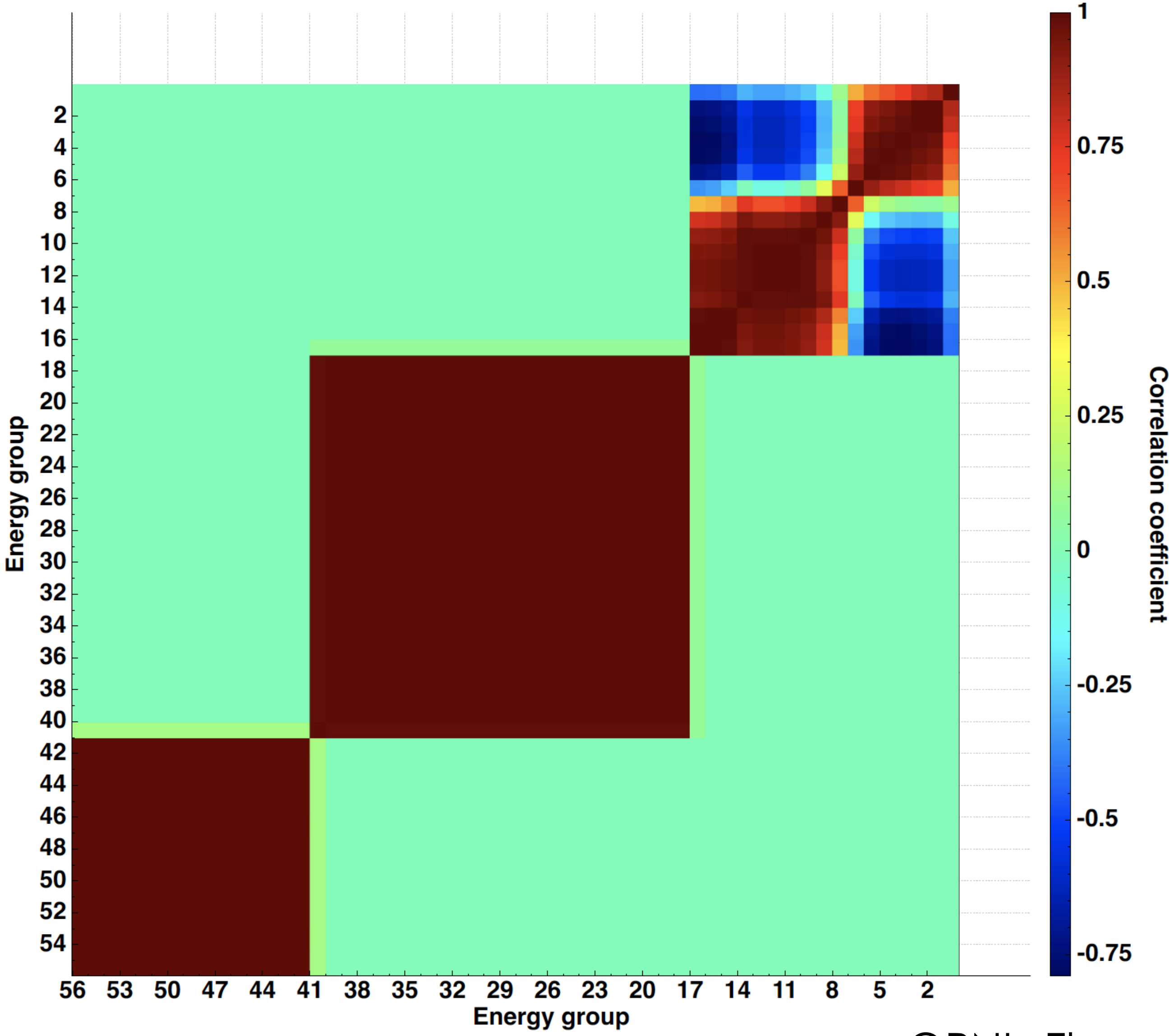
Brief history of covariance data in SCALE

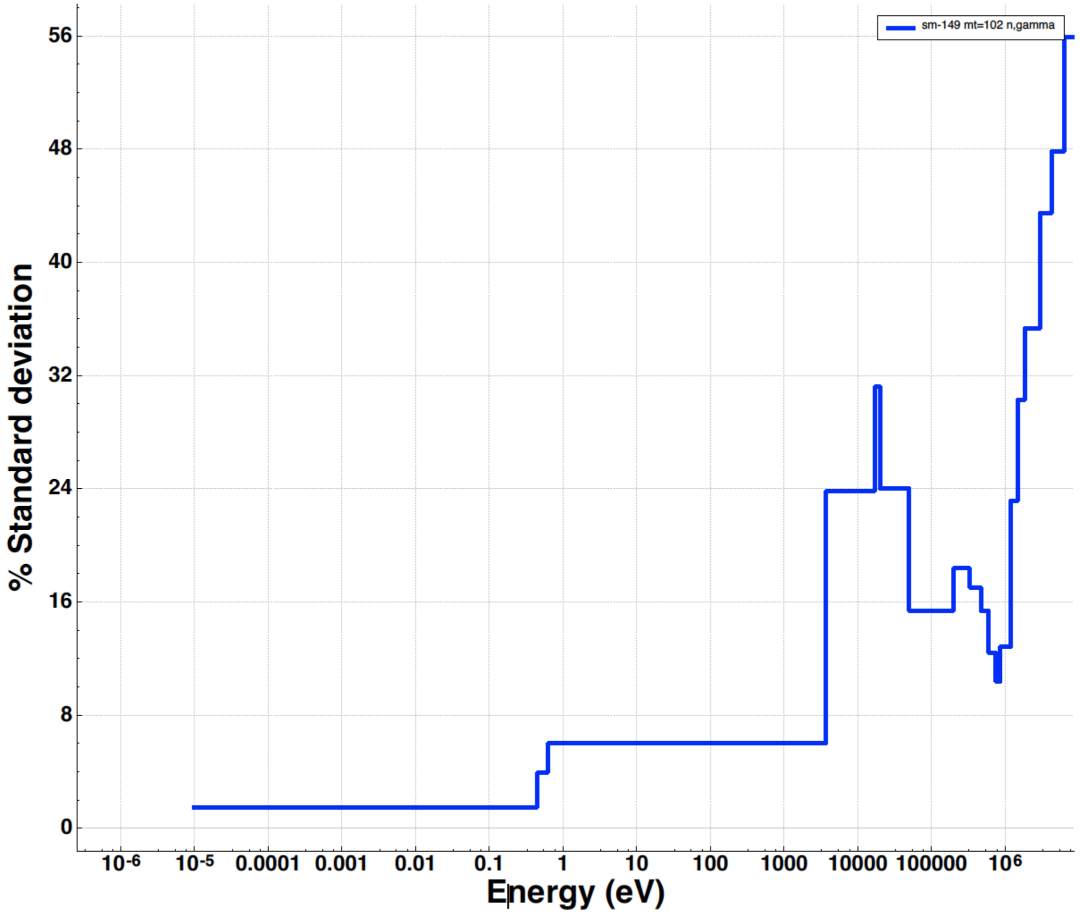
- SCALE-6
  - Creation of an applications-oriented covariance library
  - Franken-library
    - ENDF-7.0, ENDF-6, JENDL, BNL-LANL-ORNL (BLO) data
      - ORNL covariances based on the integral approximation below 5 keV
      - BNL/LANL above 5.0 keV
  - Importantly, gives SOME justifiable estimate for all materials (~277 mats)

SCALE 6.3

- ENDF-7.1
  - Covariance data for 190 isotopes
- ENDF-8.0
  - Covariance data for 251 isotopes
- Still patched with BLO data

BLO data still in SCALE covariance library (^{149}Sm, capture)





ORNL: Thermal+Epithermal- Atlas of Neutron Resonances
BNL/LANL: Fast – Nuclear Models

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Updates pursued beyond just cross sections in SCALE 6.2

#	Nuclei	Year	Author(s)
1	$^{227,229,232}Th$	1994	England et al. [1994]
2	^{231}Pa	1994	England et al. [1994]
3	$^{232-238}U$	1994	England et al. [1994]
4	$^{237,238}Np$	1994	England et al. [1994]
5	$^{238-242}Pu$	1994/2011	England [1994]/Chadwick [2011]
6	$^{241,242m,243}Am$	1994	England et al. [1994]
7	$^{242-248}Cm$	1994	England et al. [1994]
8	$^{249,251}Cf$	1994	England et al. [1994]
9	^{254}Es	1994	England et al. [1994]
10	^{255}Fm	1994	England et al. [1994]

In 1993 T. R. England and B. F. Rider produced a recommended set of *independent* and *cumulative* yields for the fission products based on a compiled list of open literature measurements and calculated charge distributions.

Except for ^{239}Pu, England and Rider FPY evaluations are still in ENDF/B-VII.1 library

Since 1993 decay sub-library data (branching ratios) updated!!

Decay data and (stable) cumulative FPY

Black dots : ratio of cumulative FPYs obtained by independent FPY and decay data in ENDF/B-VII.1 to cumulative FPYs in ENDF/B-VII.1.

Although deviations are small, **ratios should be one!!**

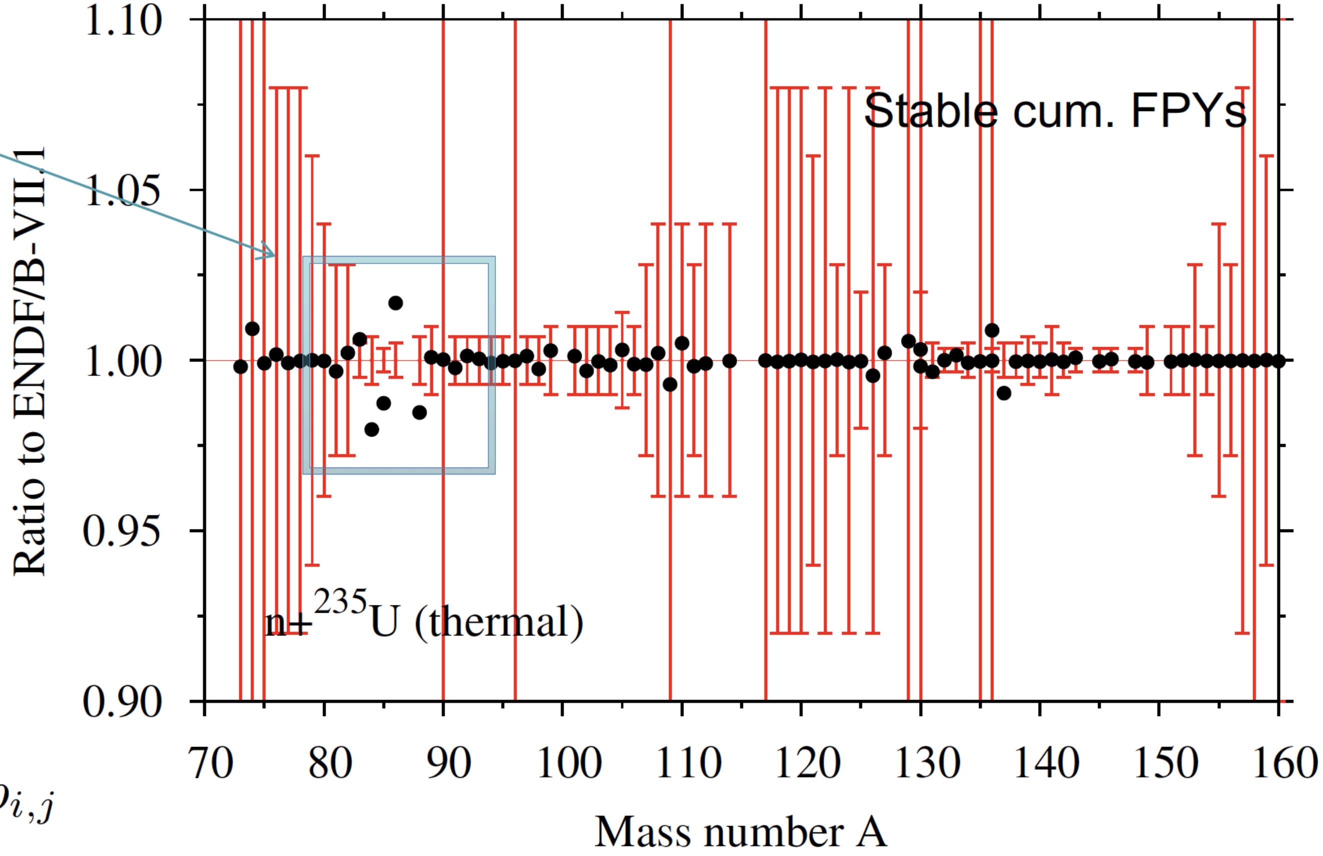
In red uncertainties (%) of cumulative yields in ENDF/B-VII.1

Biggest deviations

Cumulative yields

Independent FPY

Branching ratios



$$C_i(\mathbf{I}) = I_i + \sum_{j \in \mathbf{k}^i} C_j(\mathbf{I})\ b_{i,j}$$

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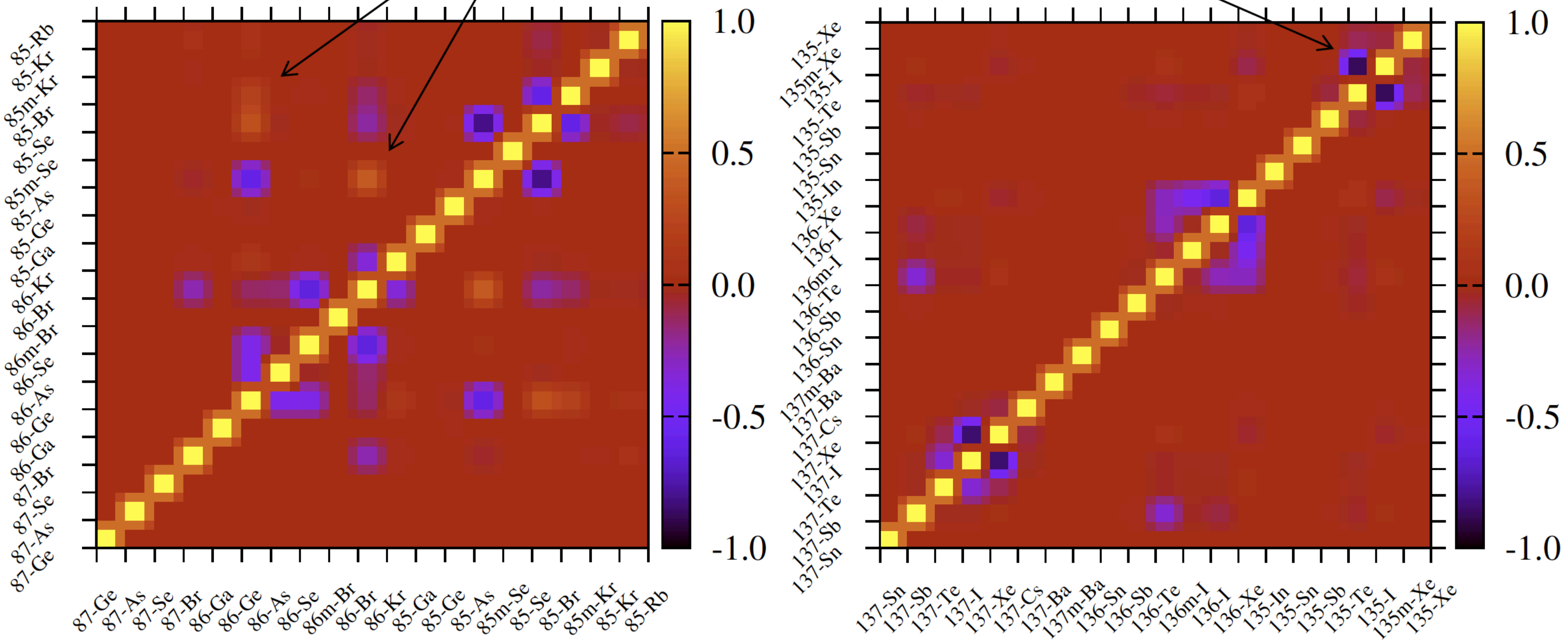
Krypton and Xenon Covariance Data

- **Strong negative correlations**
- **Relative strong positive correlations (delayed-neutrons)**



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Ramifications - LWR UAM dependent on SCALE covariances

Table I. Summary of submitted results of standalone neutronics cases.

Case	Contributor	NDL	Transport Code	VCM	UQ Method	PWR Cases	BWR Cases	VVER Cases
1	NINE	ENDF/B-VI	SERPENT 2	SCALE 6.0	Deterministic	I-1, I-2	I-1	I-1
2	EK	ENDF/B-VI	MULTICELL	SCALE 5.1	Deterministic	I-1, I-2	I-1	I-1, I-2, I-3
3	KIT	ENDF/B-VII.0	XSDRNPM	SCALE 6.1	Deterministic	I-1	I-1	I-1, I-2
4	VTT	ENDF/B-VI	CASMO-4	SCALE 6.0	Deterministic	I-1, I-2, I-3	I-1, I-2	
5	PSI	ENDF/B-VII.RO	CASMO-5MX	SCALE 6.0	Sampling	I-1, I-2	I-1, I-2	
6	NESCA	ENDF/B-VII.0	NEWT	SCALE 6.1	Deterministic	I-1, I-2, I-3	I-1	
7	UPM	ENDF/B-VII	MCNP5	SCALE 6.0	Deterministic	I-1	I-1	
	UPM	ENDF/B-VII.0	NEWT	SCALE6.1.3	Deterministic	I-2	I-2	
8	McMaster (Polaris)	ENDF/B-VII.1	POLARIS	SCALE 6.2	Sampling	I-1	I-1	
9	McMaster (NEWT-252G)	ENDF/B-VII.1	NEWT	SCALE 6.2	Sampling	I-1	I-1	
10	McMaster (NEWT-238G)	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling	I-1	I-1	
11	NRA	JENDL-4.0	CASMO5	JENDL-4.0	Sampling	I-1, I-2, I-3	I-1, I-2, I-3	
12	NWU	ENDF/B-VII.0	NEWT	ENDF/B-VII.1	Deterministic	I-1		I-1
13	SNU	ENDF/B-VII.1	McCARD	ENDF/B-VII.1	Deterministic	I-1	I-1	I-1
14	UNIST (MCS-44G-ENDF71)	ENDF/B-VII.1	MCS	ENDF/B-VII.1	Deterministic	I-1		
15	UNIST(MCS-44G-SCALE61)	ENDF/B-VII.1	MCS	SCALE 6.1	Deterministic	I-1		
16	UNIST (STREAM-GPT-56G-SCALE62)	ENDF/B-VII.1	STREAM	SCALE 6.2	Deterministic	I-1		
17	UNIST (STREAM-GPT-ENDF71)	ENDF/B-VII.1	STREAM	ENDF/B-VII.1	Deterministic	I-1		
18	UNIST (STREAM-SS-ENDF71)	ENDF/B-VII.1	STREAM	ENDF/B-VII.1	Sampling	I-1		
19	GRS (PT44G)	ENDF/B-VII.0	NEWT	SCALE 6.1	Deterministic	I-1, I-2	I-1, I-2	I-1, I-2
20	GRS (PT56G)	ENDF/B-VII.1	NEWT	SCALE 6.2	Deterministic	I-1, I-2	I-1, I-2	I-1, I-2

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LWR UAM dependent on SCALE covariances cont'd

Case	Contributor	NDL	Transport Code	VCM	UQ Method	PWR Cases	BWR Cases	VVER Cases
21	GRS (SS44G-HELIOS)	ENDF/B-VII.1	HELIOS2	SCALE 6.1	Sampling	I-1, I-2	I-1, I-2	I-1, I-2
22	GRS (SS44G-NEWT)	ENDF/B-VII.0	NEWT	SCALE 6.1	Sampling	I-1, I-2	I-1, I-2	I-1, I-2
23	GRS (SS56G-NEWT)	ENDF/B-VII.1	NEWT	SCALE 6.2	Sampling	I-1, I-2	I-1, I-2	I-1, I-2
24	ORNL	ENDF/B-VI	NEWT	SCALE 6.1	Deterministic	I-1, I-2, I-3	I-1, I-2	
25	JacobsAFW	JEFF-3.1.2	WIMS	Mixed[1]	Sampling		I-1, I-2,I-3	
26	UPV	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling	I-2	I-2	
27	Wood	JEFF-3.1.2	WIMS	WIMS	Sampling		I-3	
28	EK (Manu)	ENDF/B-VI	MULTICELL	SCALE 5.1	Sampling	I-2		
29	UPM (Sampler)	ENDF/B-VII.1	NEWT	SCALE 6.2	Sampling	I-2		
30	UPM- COBAYA without ADF	ENDF/B-VII.1	NEWT/COBAYA	SCALE 6.2	Sampling	I-3		
31	UPM -COBAYA with ADF	ENDF/B-VII.1	NEWT/COBAYA	SCALE 6.2	Sampling	I-3		
32	NESCA	ENDF/B-VI	MGRAC	SCALE 6.1	Sampling	I-3		
33	UPM COBAYA pin-by-pin	ENDF/B-VII.1	NEWT/COBAYA	SCALE 6.2	Sampling	I-3		
34	UPM COBAYA nodal	ENDF/B-VII.1	NEWT/COBAYA	SCALE 6.2	Sampling	I-3		
35	THU (REAL)	ENDF/B VII.0	RMC	SCALE 6.0	Sampling	I-3	I-3	
36	NCSU	ENDF/B-VII.1	POLARIS	SCALE 6.2	Sampling	I-3		
37	NCSU (MPACT)	ENDF/B-VII R1	MPACT	ENDF/B-VII.1	Sampling	I-1, I-2	I-1, I-2	

29 out of 37 participants using SCALE covariance!!

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6.3 Goals

- delayed neutron uncertainty
- sensitivity indices
- improved infrastructure for covariance operations
- on-the-fly sampling and correlated input sampling

Unexpected Uncertainty:

- Delayed neutron fraction, arguably one of most important safety parameters

$$\frac{dn(t)}{dt} = \frac{\rho-\beta_{eff}}{\Lambda} n(t) + \sum_{i=1}^{N} \lambda_i C_i(t)$$

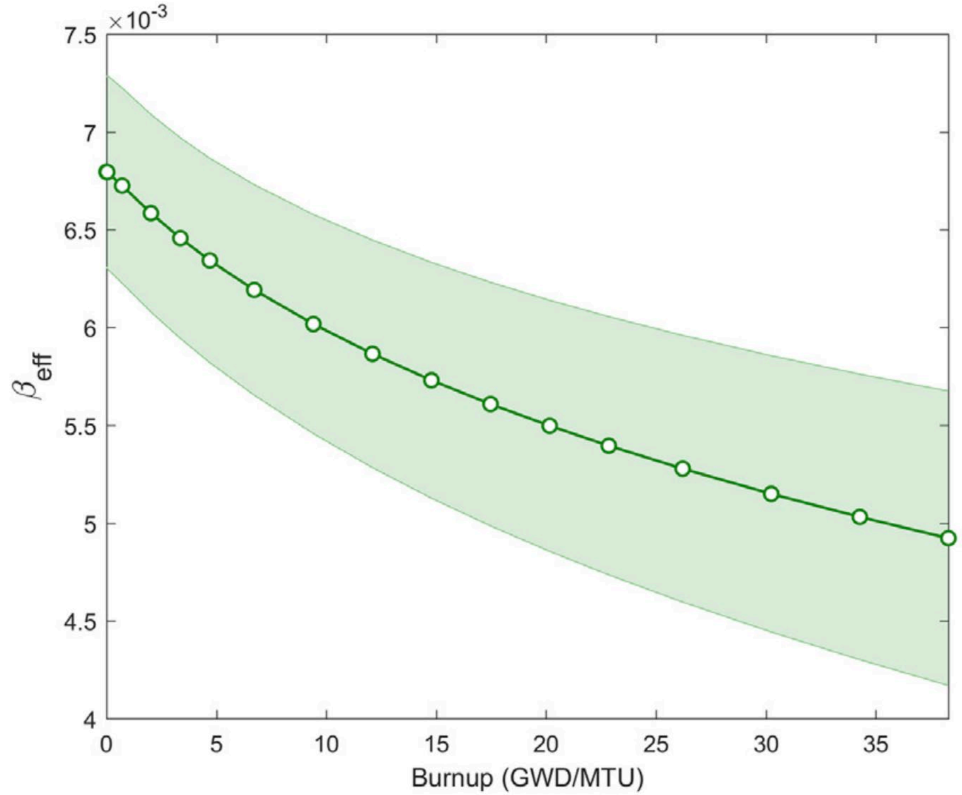
$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t), \qquad (i = 1, \ldots, N)$$

- **For LWR systems**: SCALE/Sampler uncertainty propagation of just **cross sections**
  - Fresh fuel: β_{eff}~700 pcm +/- 7%
  - 40 GWd/MTU: β_{eff}~500 pcm +/- 15% (2-sigma range is 350-650 pcm)

- Is it real?
  - Sampling error?
  - Neglected correlation?
  - **As we investigate non-LWRs, need perspective**

$$\beta_{eff} = \sum_{i=1}^{6} \frac{\sum_j \sum_m V_m (\sum_g \nu\sigma_{fjgm} n_{jm} \phi_{m,g})(\sum_{g'} \beta_{g'ji}\, \chi_{d,g'mj} \phi^*_{g'm})}{\sum_j \sum_m V_m (\sum_g \nu\sigma_{fjgm} n_{jm} \phi_{m,g})(\sum_{g'} \bar{\chi}_{g'mj} \phi^*_{g'm})}$$

j – fissionable nuclide
m – material
i – delayed neutron group



Majdi I. Radaideh, William A. Wieselquist, Tomasz Kozlowski, "A new framework for sampling-based uncertainty quantification of the six-group reactor kinetic parameters", *Annals of Nuclear Energy*, Volume **127** (2019).

Sensitivity Indices

- Sampler able to report new sensitivity indices
  - squared multiple correlation coefficient R^2
    - expected amount by which the total **output** variance would be reduced in case the true values of the **input** parameter group would become known
  - semi-partial squared multiple correlation coefficient SPC^2
    - describes the variance of the **output** quantity which is expected to remain when the true values of the complementary parameter group became known
  - New indices can be used for any output response (e.g. k-eff)

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Unifying linear algebra and matrices

- Historically the SCALE code base was littered with a myriad of different matrix and linear algebra implementations
  - Costly maintenance, requires developers to rebuild mental models as they work in different parts of the code

- Robust linear algebra and matrix packages exist BUT
  - Steep learning curves
  - Unstable or too problem domain specific
  - Outpaced by new software

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Unifying linear algebra and matrices

- We are developing an interface layer between the details of a specific linear algebra and matrix implementation and SCALE
  - Current target is wrapping Trilinos
  - Interface future proofs SCALE
    - One place to swap out implementation details
    - Reusable everywhere in SCALE (and AMPX, SAMMY, etc.)

- Currently targeting sparse matrix implementations
  - Developing high-level linear algebra routines that take the interface layer as arguments
  - Allows SCALE implementation to grow organically with developer and sponsor needs

on-the-fly sampling and correlated input sampling

- We have the technology…
- Long term vision
  - We already generate samples from the covariance matrices, but ideally we should be able to sample from them on-the-fly to remove the current 1000 realizations limit
  - Investigate sampling methods, storage methods, and representations
  - Modifying our covariance data resources to be more flexible for different quantities of interest

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Questions?

- Thanks to our sponsors!
  - NCSP
  - NRC
- Thanks to colleagues and collaborators!
- Tutorial in next session
  - Generation of SCALE Multigroup Libraries for Advanced Reactors using AMPX
- Upcoming Fall Training – Nuclear Data **Fun**damentals and AMPX Library Generation
  - October 26-28, 2020
  - Description: https://www.ornl.gov/scale/scale/nuclear-data-fundamentals-and-ampx-libraries-generation-course

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